Molecular simulation of complex transitions

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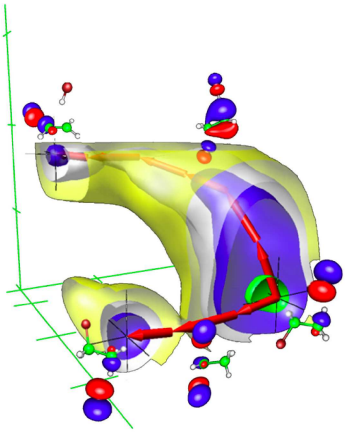

The motions of atoms and molecules nowadays be visualized with accur computer simulations that are based on sta of-the-art quantum-chemical calculations carefully parameterized force-fie Simulations give us unique insight in microscopic behavior of materials and prov an important tool to interpret spectrosco and other experiments. There is one cav however: almost all (bio-) chemical proces (think of chemical reactions, phase transitic proteins folding, molecular self-assembly, a so forth) take place on time scales that much longer than the femtosecond time sc of the atomic motions. In other words, these activated processes are (very) rare events during the relatively short molecular simulations.

In this talk, I will explain how molecular transitions can be seen as trajectories through a (free) energy landscape with valleys, mountains and connecting passes. Using special techniques, such as our recently developed "path-metadynamics method", we can sample these reactive trajectories, visualize the free energy landscape and discover the reaction mechanisms that underlie the experimentally measured reaction rates. I will illustrate these powerful simulation techniques with examples from organic and bio-chemistry, electron transfer processes and signal propagation in photo-active proteins.